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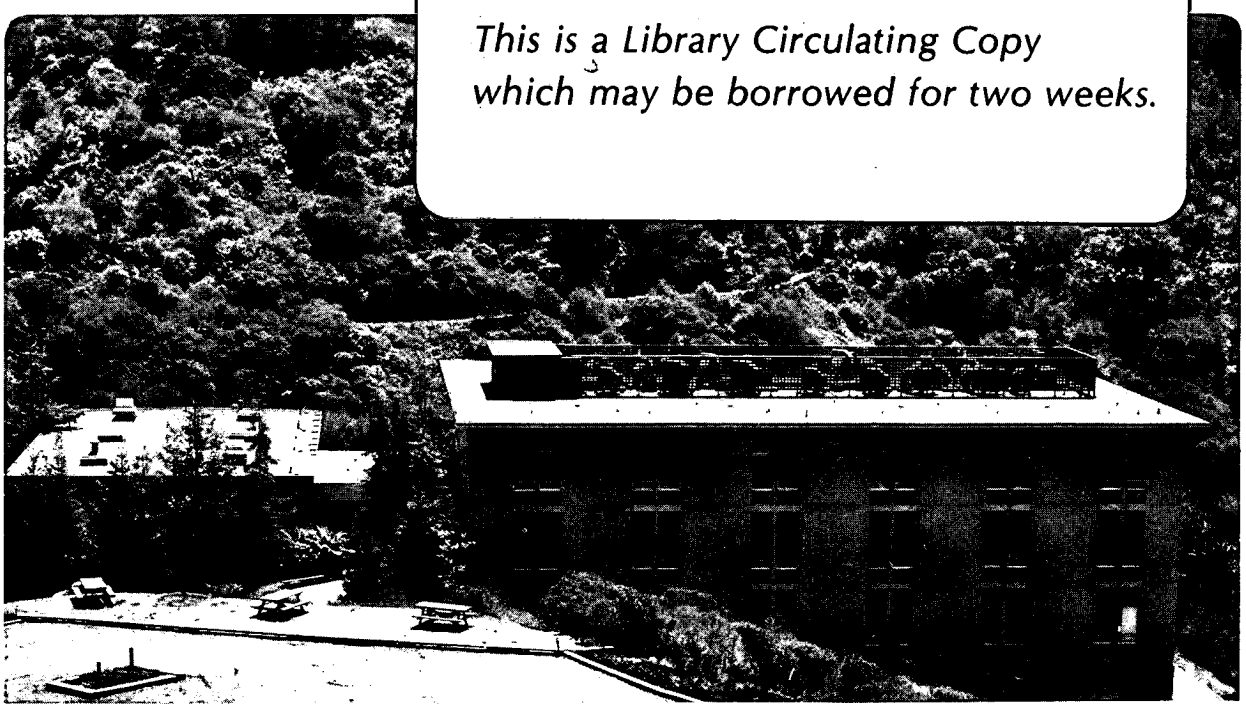

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DISCLAIMER

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ON THE USE OF CONVERGENT BEAM ELECTRON DIFFRACTION FOR IDENTIFICATION OF ANTIPHASE BOUNDARIES IN GaAs GROWN ON Si

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INTRODUCTION

The growth of GaAs on Si has been recognized as a highly desirable technology goal for a number of years.[1,2] However, the large lattice misfit between GaAs and Si and the problem of growing a polar crystal on a nonpolar substrate can result in a high density of lattice defects, including antiphase disorder. At an antiphase boundary (APB) the Ga-As bonds are replaced by As-As and Ga-Ga bonds. It is expected that APBs can be highly charged, and they might collect charged impurities unless As-As and Ga-Ga bonds are so close that they can neutralize each other.[3] APBs can result from the coalescence of GaAs domains independently nucleated on the Si substrate. This can occur due to a single (a/4) Si surface step (or an odd number), or when the coalescing domains have grown so that one domain starts with a Ga layer and the other domain starts with an As layer. It was shown[4] that As has a strong affinity for the Si (001) surface, and GaAs grown on Si usually starts with As-Si bonds, but there is some evidence that a first Ga layer can be formed when deposition is done at high temperature with low As flux.[5] High temperature treatment is used in order to remove residual oxide from a surface, but its removal may be incomplete. This treatment can also result in small steps or in a change in composition of the first layer. It was also suggested that both types of steps (single and double) are distributed equally on the Si substrate before GaAs growth, and a choice of step site and orientation for nuclei is governed by the most energetically favored configuration.[6] This sugestion permits the conclusion that the formation of antiphase disorder is dependent on the growth conditions.

In addition, it has been claimed that the substrate orientation might play a crucial role in the

formation of APBs.[1,7] Slight tilting from [001] toward [110] or [110] increases the density of one type of steps, which are oriented along [110] or [110], respectively. This tilting reduces the terrace width between steps over which atoms must move to reach the steps and thereby reduce the time required to form a primitive surface (a/2 steps), thus avoiding the formation of APBs.[7]However, real surfaces, even with off (001) orientations, have a residual angular deviation that might be inhomogenous across the Si wafer and thus act as an additional source of APBs.[8]

A possible solution to this problem is the use of Si (211) surfaces, which, because of their nonpolar character, do not form APBs.[1] However, such a substrate orientation promotes the propagation of threading dislocations from the GaAs/Si interface[9] and moreover would require a modified Si technology. Another way to reduce the density of APBs is to grow thick GaAs layers, which have been shown to result in the annihilation of some APBs.[1,10] But growth of too thick GaAs layers increases the problems connected with different thermal expansion coefficents, so that a final solution can only come from a thorough understanding and control of the formation of antiphase disorder during the initial stages of epitaxy. The electron microscopy studies necessary to reach this goal require the ability to indentify antiphase disorder in situ in the electron microscope , especially near the hetero-interface, where chemical etching,which is usually used to indentify the presence of antiphase disorder, fails.

This paper utilizes Convergent Beam Electron Diffraction (CBED) patterns, which allow tone o identify the crystal polarity[11] for the investigation of APBs.

DETERMINATION OF CRYSTAL POLARITY

CBED has been shown to detect polarity of a compound crystal in a TEM sample.[12] The coupling between the (200) reflection and weak odd-index reflections in the Bragg position gives a special pattern (cross) in the (200) and (200) discs that is sensitive to the order of the As and Ga planes in the sample. It was shown that a white cross in the (200) CBED disc obtained in a Phillips 400 T electron microscope with 100KeV acceleration voltage was correlated with As

planes oriented 55° clockwise from the particular (200) direction, and a black cross in the same disc was associated with Ga planes in the same crystallographic orientation as the As. In this way it is easy to check the polarity of particular regions in the sample in situ in the electron microscope. In this paper the method is applied to detect the presence of APBs in GaAs grown on Si.

EXPERIMENTAL

GaAs crystals of ~ 1um thickness were grown by Metalorganic Chemical Vapor Deposition (MOCVD) on (001) Si substrates that were not intentionally tilted. Cross-sectional samples along Si [110] and [100] were prepared for TEM observation with the conventional "sandwich" technique. Specimens were ion milled in order to obtain samples transparent to electrons. The samples were examined in a JEOL JEM-200CX (200kV) high resolution electron microscope, the Atomic Resolution Microscope (ARM) and a Phillips 400 T (100kV) in order to obtain the CBED patterns needed to determine the presence of APBs.

RESULTS AND DISCUSSION

All cross-sectional samples had a very high density of defects in the GaAs layer (Fig. 1). Many twins and stacking faults propagated from the interface to the surface of the GaAs layer. Some of them annihilated at a distance of several nanometers from the interface, but many defects stopped at faint lines along which the contrast became fringe-like. A similar fringe-type contrast was observed by Carter et al[13,14] and identified as an APB. As can be seen in Fig. 1 such a fringe-like boundary extended through a large area of the sample.

To ensure that the observed contrast is associated with APBs the sample was placed in the Phillips 400 T electron microscope, where a CBED pattern was taken on both sides of the boundary. The sample was tilted to fulfill the condition of coupling two odd reflections, 715 and 915, with the 200 reflection. A black cross was observed in the 200 disc, which changed to

white when the beam was placed on the opposite side of the boundary (Fig. 2). This confirms that the stacking order has been changed on the (111) planes across the boundary. This change can be associated only with the presence of an APB.

Faceting of APBs was commonly observed. It can be seen in Fig.2 that part of the APB is parallel to (110) and another part appears to be parallel to (111) (as are the twins which can be seen in this figure).On closely inspection, the part of the APB that appears to be parallel to (111) is composed of small regions of {110} boundaries viewed either edge-on or inclined to the surface. This faceting on {110} can be seen even more clearly in Fig. 3 where the entire boundary is on average parallel to (111), but small sections are {110} planes viewed either edge-on or inclined (visible as ribbons). This faceting is probably driven by minimalization of interfacial energy. This observation is in agreement with Petroff's[15] prediction that (110) APBs have the lowest interfacial energy . Such APBs contain alternate Ga-Ga and As-As bonds, thus minimizing interfacial charges. It can be seen in Fig. 2 that the GaAs crystal was growing faster on one side of the APB than on the other side of the APB (see the step on the crystal surface indicating different thickness) of the GaAs. Failure of this boundary to continue the original direction is another indication of the anisotropy of APB interfacial energy favoring {110} APBs.

APBs effectively stop the propagation of twins and stacking faults (Figs.1 and 4). This demonstrates the severity of lattice disorder connected with an APB, which can be regarded as a special case of a grain boundary.

Most APBs propagate to the surface of the GaAs layer (Figs.1, 2, and 3) but in some places anihilation of APBs was observed (Fig. 5). However, the anihilation mechanism seems to be more complicated than the one described by Kawabe et al.[10] Faceting on the energetically favorable {110} planes rather than on the suggested {111} planes[10] dominates in this case as well.

It is difficult to decide if these APBs are the result of odd surface steps on the Si surface or due to domain growth with both As-Si and Ga-Si bonding on the GaAs/Si interface, because of the presence of a ~0.2 nm thick layer on the interface. This 0.2 nm layer did not show lattice images in either the (100) or in (110) projection, even in the ARM, with a point -to-point

resolution of 1.6 Å. This amorphous layer has been observed by other reaserchers as well.[16] It is not likely that this amorphous layer is connected with the TEM sample preparation, because an extended study of metal samples deposited in situ in UHV on cleaved GaAs surfaces with identical TEM sample preparation (including ion milling) never resulted in the formation of such an amorphous layer. However, amorphous layers were observed for samples with metal deposited on air exposed GaAs surfaces.[17] Therefore it is assumed that this amorphous layer was some kind of contamination present on the Si surface prior the GaAs growth. It was observed that APBs were more common in areas where larger contamination agglomerations were present (Figs. 4 and 6).

CONCLUSIONS

This study shows that dynamical coupling effects in CBED patterns can be unambiguously used to detect APBs. A high density of APBs can be present in GaAs grown by MOCVD on Si (100) surfaces. APB formation is promoted by surface contamination and irregularities.

APBs act as natural obstacles for the propagation of twins and stacking faults into the growing epitaxial layer. Faceting of APBs is probably connected with anisotropy of the interfacial energy of APBs. In most cases extended surface areas of APBs were observed to lie on the energetically favorable {110} planes. This observation is in agreement with earlier theoretical calculations.

ACKNOWLEDGMENTS

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FIGURE CAPTIONS

Fig.1 Dark field image of the GaAs/Si interface. A fringe-like contrast of an antiphase boundary (shown on the right side of the picture where the APB is approximately parallel to the (001) plane) changing to a fine line contrast (in the middle of the picture). Note that the APB is an obstacle for all kinds of defect propagation.

Fig.2 The APB with the "average" {111} plane changing to {110}. The CBED pattern was taken on both sides of the APB in the areas marked by circles. The black cross is seen in the 200) disc when beam is on the left side of the APB, and the white cross is seen in the (200) disc when the beam is on the right side of the APB (see inserts). This indicates that the same (111) plane is occupied by Ga on one side of APB, changing to As on the other side of the APB.

Fig. 3 The APB composed of small facets along {110} planes (edge-on or inclined) which ,when viewed as a whole, appears as an average plane of {111} parallel to the twin plane shown in the picture.

Fig.4 High resolution image of the APB in the {110} projection. Note the interaction of a twin with the APB and an impure amorphous layer at the interface which can be considered as an additional source of defect nucleation.

Fig.5 The antiphase domain in GaAs grown on Si. Anisotropy of APB formation energy promotes faceting, leading to an annihilation of APB.

Fig.6 High resolution image of the APB taken in the {100} projection. Note that impurity agglomeration on the interface with Si favors nucleation of the APB.

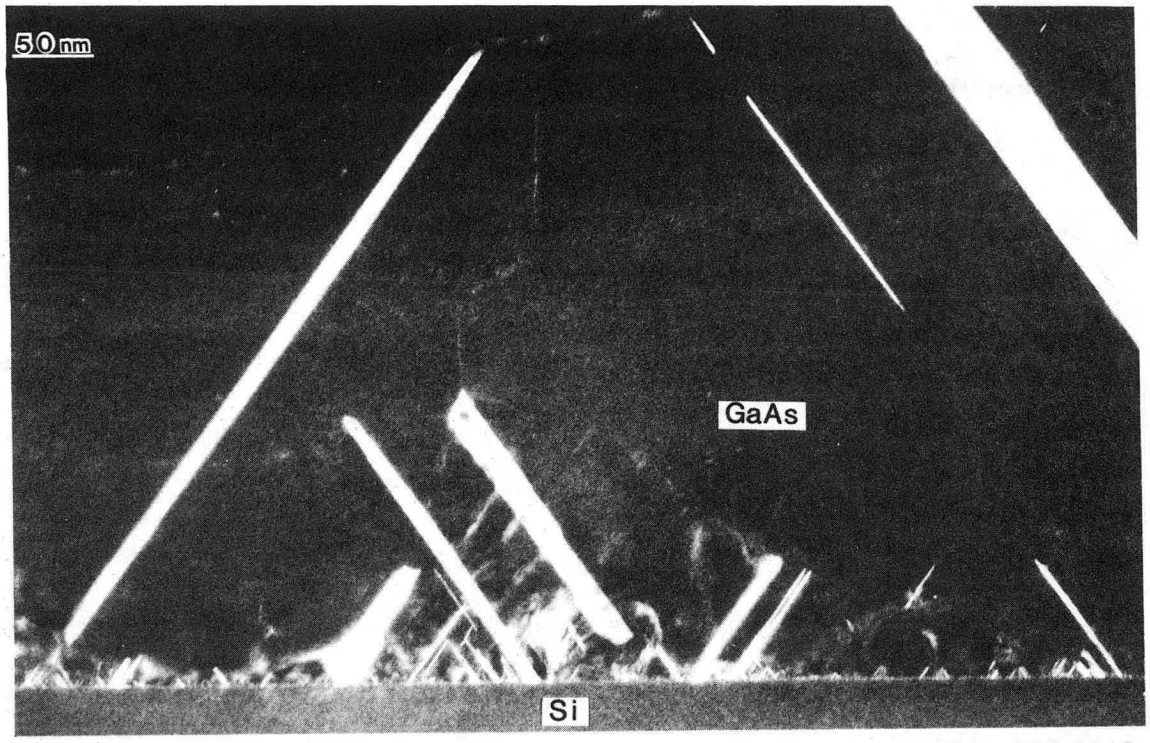

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Fig. 1

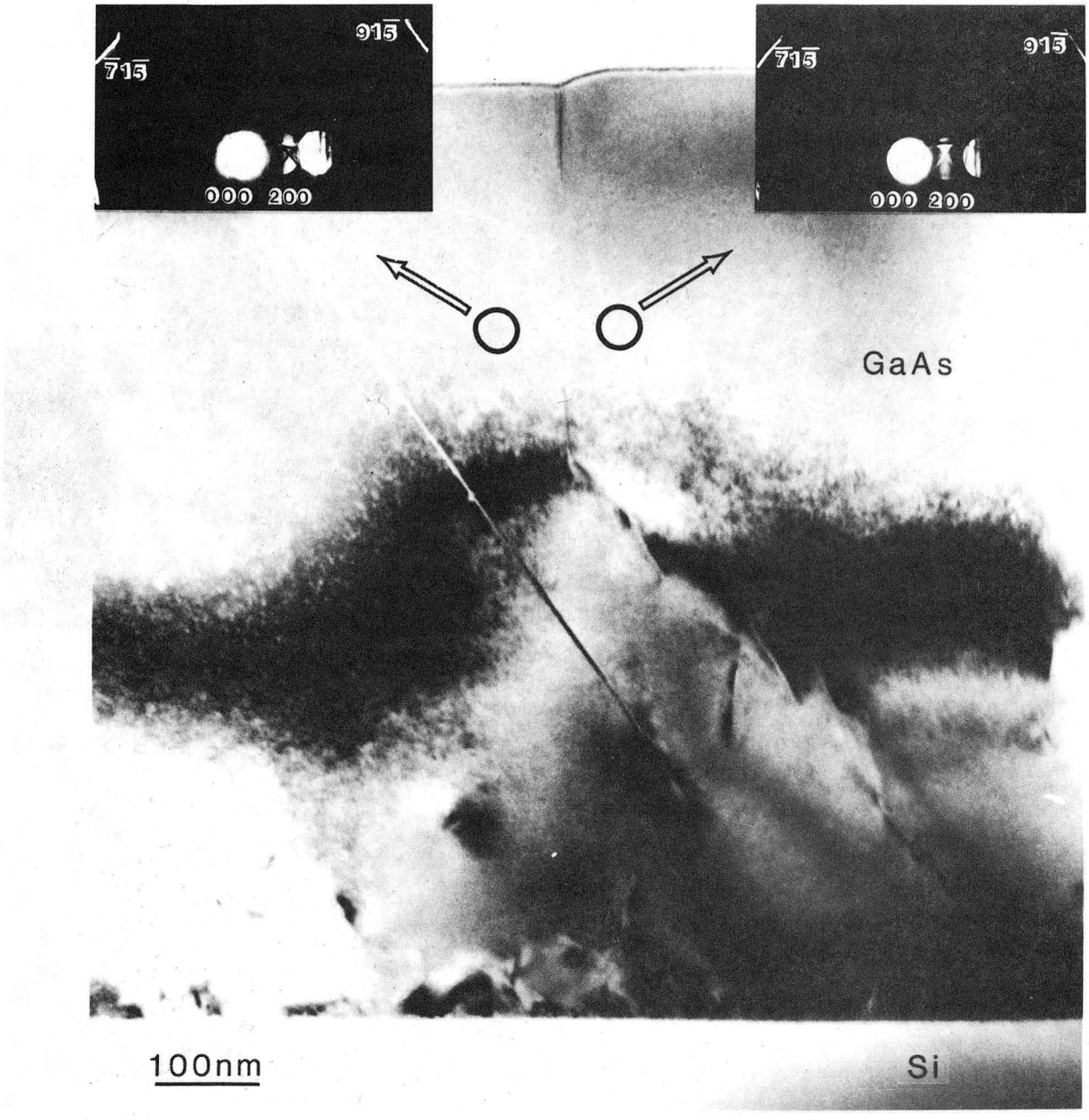

Fig. 2

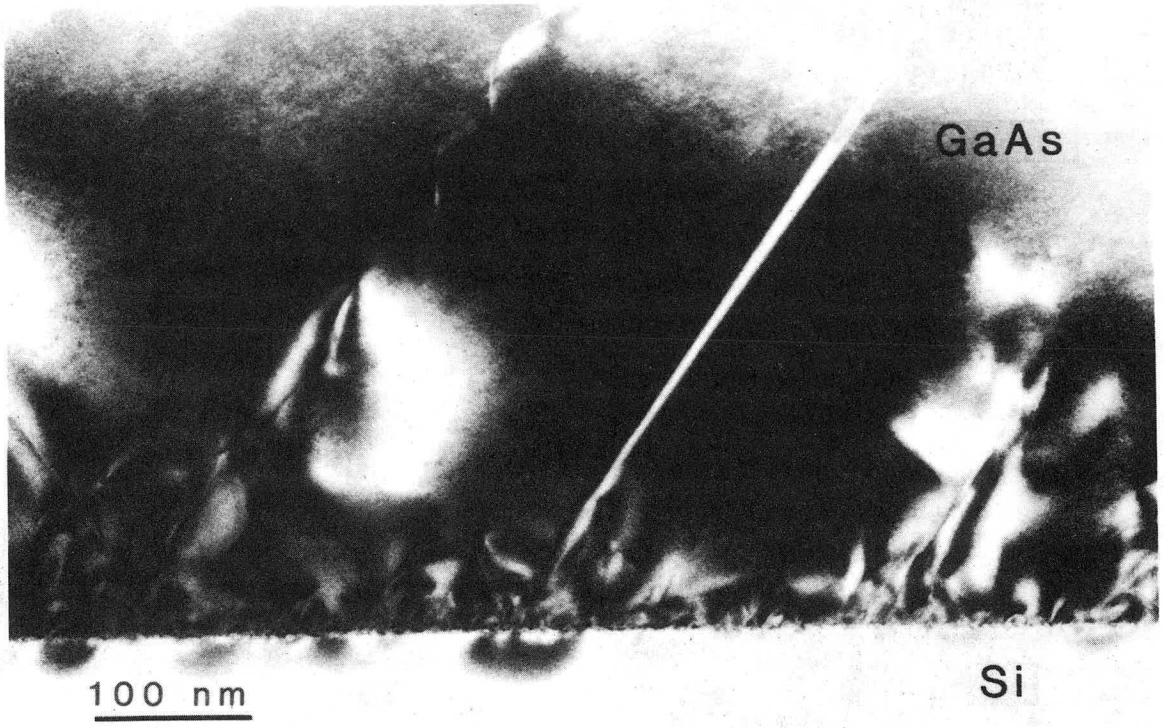

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Fig. 3

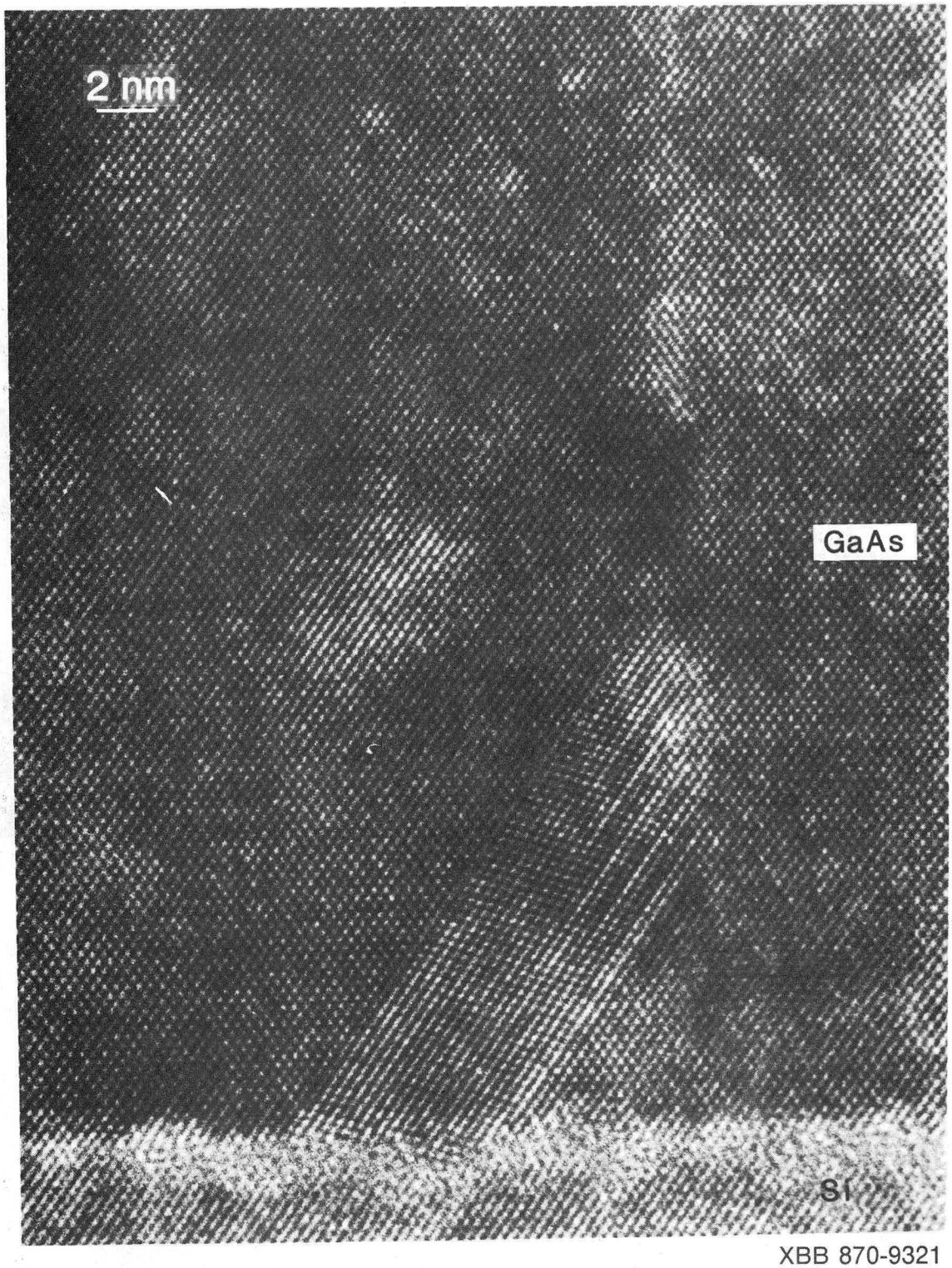

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Fig. 4

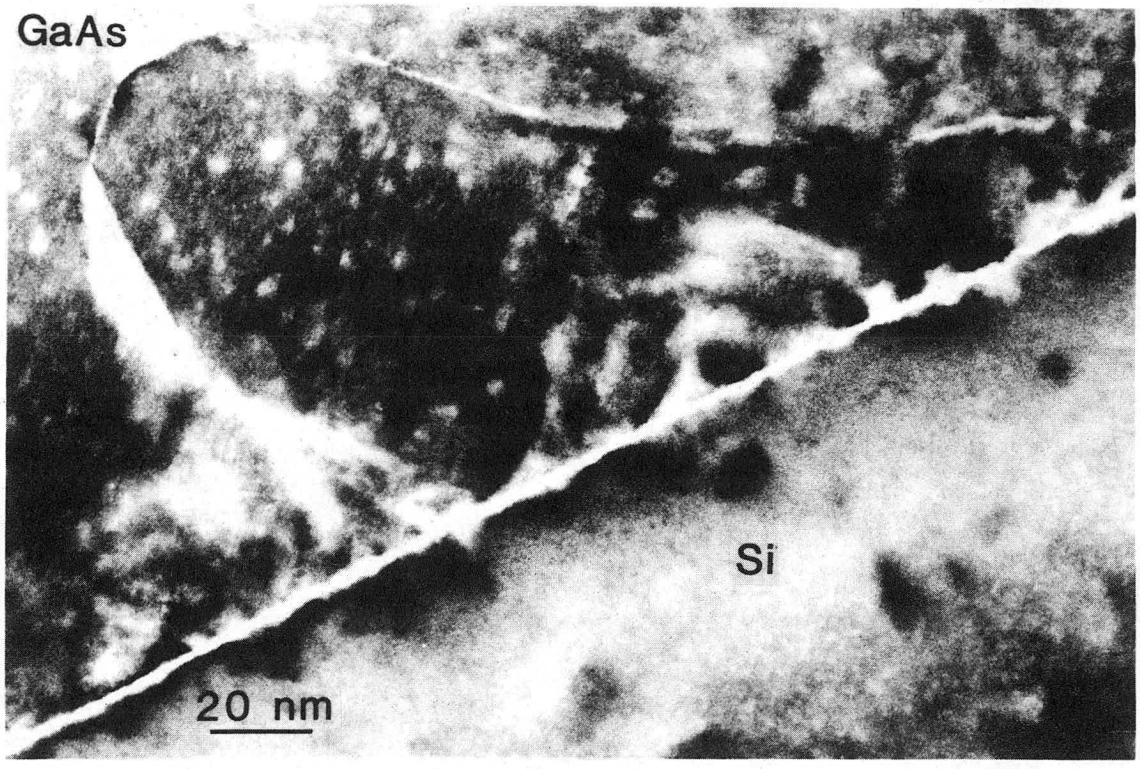

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Fig. 5

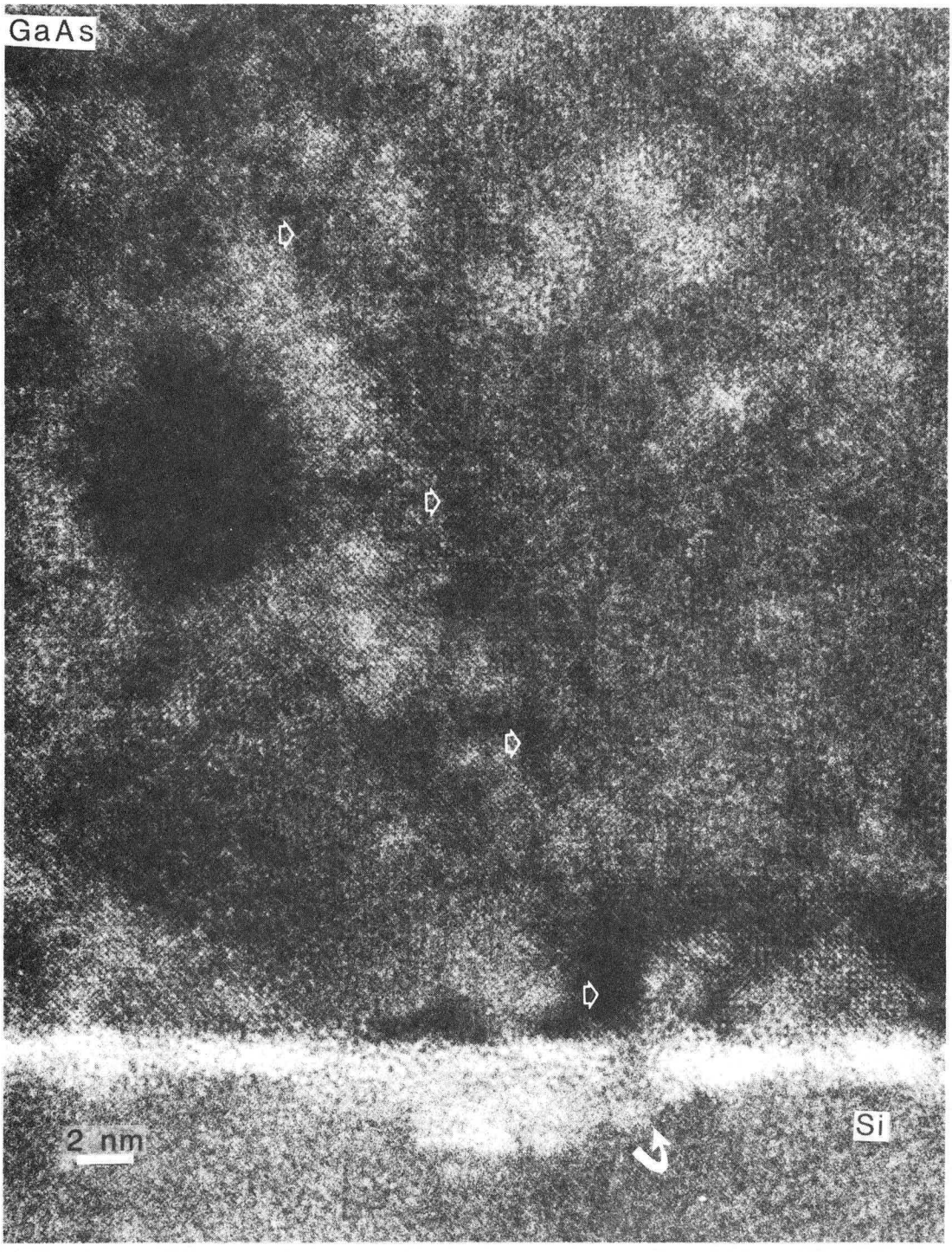

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Fig. 6

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